Supporting Information

Synthesis of α-hydroxy threonine (Tah, 2*R*, 3*S*-dihydroxy-butanoic acid) (1). L-Threonine (2.2 g, 18.5 mmol), suspended in 5 ml of water at -5 °C, was treated simultaneously with a solution of 1.38 g $NaNO_2$ (20 mmol) in 2 ml of water and 557 µl of concentrated H_2SO_4 (10 mmol) in 1.5 ml H_2O. The two solutions were added slowly while stirring so that the temperature remained between 0 °C and 5 °C. The reaction turned yellow upon addition. The solution was then stirred overnight at room temperature. The reaction mixture was concentrated, the mixture treated with 3 ml of EtOH, and the salts were filtered. The solution was concentrated. The material was dry loaded onto a flash silica gel column and run in 1:1 hexanes/ethyl acetate with 1% acetic acid to give 730 mg (38 %) of hydroxythreonine: ^{1}H NMR (D_2O) δ 1.17 (d, 3 H, J = 6 Hz), 4.1 (m, 2H); ^{13}C NMR 18.2, 68.4, 74.2, 176.0: FAB MS Calcd for $C_4H_9O_4$ plus H: 121.0501. Found *m/z:* 121.0470.

Synthesis of Tah cyanomethyl ester (2*R*, 3*S*-dihydroxy-butanoate cyanomethyl ester) (2). The hydroxy acid (385 mg, 3.21 mmol) was dissolved in 5.1 ml of $ClCH_2CN$ (80.1 mmol) and 1.2 ml Et_3N (8.44 mmol). Upon stirring under Ar for 30 min, the solution turned yellow. A gradient flash silica gel column from 20% to 80% ethyl acetate/hexanes was run, and the isolated product was dried on vacuum to yield 50.9 mg (10%) of hydroxythreonine cyanomethyl ester: ^{1}H NMR (D_2O) δ 1.27 (d, 3H, J= 6 Hz), 4.22 (m, 1H), 4.34 (d, 1H, J= 3 Hz), 5.01 (s, 2H), ^{13}C 18.2, 49.7, 68.4, 74.4, 115.5, 172.6; FAB MS Calcd for $C_6H_9O_4N$ plus H: 160.17. Found *m/z*: 160.03 (M+H), 75.02, 103.07.

Table 1. Calculated Binding Energies* (kcal/mol)

Agonist	Amide Trp	Ester Trp	Ester – Amide
ACh	- 21.7	- 16.7	5.0
Nic	- 30.4	- 24.3	6.1
(+) Epi	- 34.8	- 26.6	8.2
(–) Epi	- 35.5	- 27.7	7.8

* HF/6-31G, Gas phase.

Support for the assignment of a dielectric constant of 24.3 to the nAChR binding site environment. Previous work (3) with protonatable tethered agonists in the nicotinic acetylcholine receptor binding site has shown a pK_a shift of at least 4 units. A literature survey of the pK_a shifts of organic acids and bases in water/solvent mixtures of varying dielectric constants shows that a pK_a shift of 4 units is consistent with a dielectric constant (ε) of about 25. The dielectric constant of ethanol is 24.3.

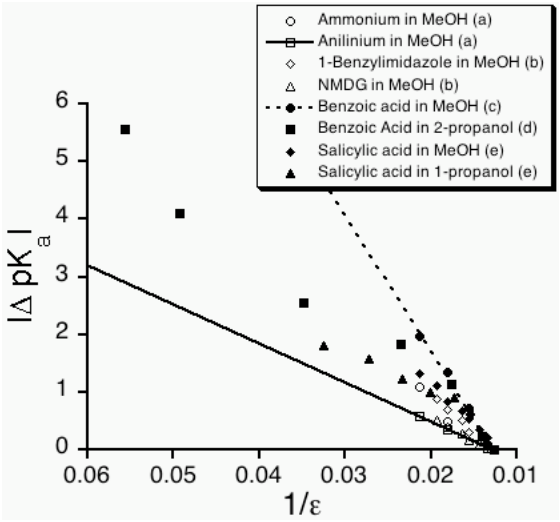

Fig 1.pK_a shifts of organic acids and bases in water/solvent mixtures of varying dielectric constants. Data from the following sources: (a) Bosch, E. *et al*. (1996) *Anal. Chem*. **68**, 3651-3657. (b) Avdeef, A. *et al*. (1993) *Anal. Chem*. **65**, 42-49. (c) Niazi, M. S. K. (1989) *Bull. Chem. Soc. Jpn*. **62**, 1253-1257. (d) Bosch, *et al*. (1995) *Analytica Chimica Acta* **302**, 109-119. (e) Niazi, M. S. K. (1993) *J. Sol. Chem*. **22**, 437-449.

[1] Servi, S. (1985) *J. Org. Chem*. **50,** 5865-5867.

[2] England, P. M., Lester, H. A. & Dougherty, D. A. (1999) *Tetrahedron Letters* **40,** 6189-6192.

[3] Petersson, E. J., Choi, A,, Dahan, D. S., Lester, H. A., Dougherty, D. A. (2002) *J. Am. Chem. Soc*. **124**, 12662-12663.

The binding site environment was investigated computationally by calculating the solvent accessible surface areas (SASA) of the residues in AChBP using NACCESS.(4) Trp 143 (Trp 149 muscle nAChR numbering) was found to be 10.8% solvent accessible. A mid-range dielectric constant of 24.3 ($\varepsilon(H_2O)$ = 78.5, ε(hydrocarbon) ~ 2) seems reasonable for a moderately accessible site such as Trp 149.

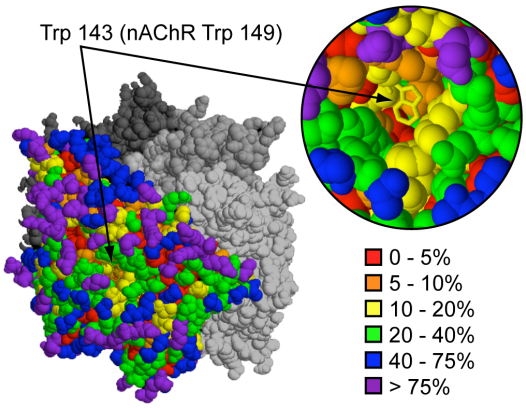

Fig. 2. AChBP residue SASA. Two AChBP subunits shown colored according to SASA. Inset shows binding site with residues 73, 106, 112, 187, 188, 189, 190, and 192 removed for clarity. Trp 143 shown as stick representation. Residue solvent accessibilities were evaluated for a solvent of radius 1.40 Å. Accessibility is defined as the percentage of sidechain surface area accessible to the probe in the protein relative to the surface area accessible in an A-X-A tripeptide.

[4] Hubbard, S. J. & Thornton, J. M. (1993) NACCESS (Department of Biochemistry and Molecular Biology, University College, London, U.K.)

HF/6-31G geometries in Gaussian "standard" orientation.

Amide

1	6	-1.672610	-1.559835	-0.325739
2	6	-2.535131	-0.633875	0.500882
3	8	-2.395842	-0.522298	1.716081
4	6	-0.861909	-0.847868	-1.432500
5	6	0.156787	0.121171	-0.910069
6	6	0.043749	1.468676	-0.836109
7	6	1.459625	-0.210436	-0.366618
8	7	1.187643	2.012479	-0.282106
9	6	2.067982	0.995913	0.014298
10	6	2.152177	-1.410650	-0.181714
11	6	3.342474	1.037026	0.575254
12	6	3.414351	-1.377688	0.372266
13	6	4.003356	-0.160517	0.748996
14	7	-3.493141	0.058494	-0.164532
15	6	-4.400096	0.958787	0.527433
16	1	-1.005191	-2.057000	0.362004
17	1	-1.534637	-0.336256	-2.113443
18	1	-0.365956	-1.611541	-2.023592
19	1	-0.768358	2.094771	-1.132976
20	1	1.335283	2.974018	-0.105934
21	1	1.711128	-2.347795	-0.464722
22	1	3.795115	1.966472	0.863835
23	1	3.956696	-2.291270	0.521789
24	1	4.985975	-0.164045	1.180275
25	1	-5.064878	0.418005	1.188457
26	1	-4.988565	1.492343	-0.205053
27	1	-3.844002	1.669482	1.121073
28	1	-3.622814	-0.093243	-1.134482
29	1	-2.309104	-2.316582	-0.777692

Ester

1	6	-1.684484	-1.577555	-0.415491
2	6	-2.513618	-0.710739	0.483565
3	8	-2.574518	-0.807227	1.691013
4	6	-0.901484	-0.793091	-1.485381
5	6	0.117099	0.150216	-0.916329
6	6	0.002745	1.494814	-0.797146
7	6	1.416704	-0.198913	-0.374618
8	7	1.142023	2.019965	-0.214704
9	6	2.021597	0.994238	0.051892
10	6	2.109995	-1.404030	-0.227304
11	6	3.292124	1.016866	0.622919
12	6	3.368284	-1.389279	0.336437
13	6	3.953194	-0.185476	0.759574
14	8	-3.251352	0.194726	-0.194077
15	6	-4.133045	1.079798	0.532457
16	1	-1.019904	-2.148157	0.216624
17	1	-1.604169	-0.247297	-2.100393
18	1	-0.410745	-1.513493	-2.132575
19	1	-0.807215	2.127710	-1.084779
20	1	1.295025	2.977060	-0.019780
21	1	1.673123	-2.330721	-0.548593
22	1	3.742287	1.936207	0.945832
23	1	3.911239	-2.306844	0.456458
24	1	4.933123	-0.202998	1.196600
25	1	-4.867965	0.507497	1.075701
26	1	-4.601874	1.690490	-0.218195
27	1	-3.565465	1.683551	1.222545
28	1	-2.359340	-2.273847	-0.905465

ACh

1	6	-2.718473	0.518649	1.224882
2	7	-1.843253	0.092946	0.069036
3	6	-1.528263	1.320023	-0.762562
4	6	-2.595107	-0.912825	-0.763243
5	6	-0.577083	-0.518292	0.649577
6	6	0.379345	-1.123445	-0.385577
7	8	1.729726	-0.989025	0.084883
8	6	2.357284	0.216056	-0.044646
9	6	3.788800	0.163141	0.347961
10	8	1.738011	1.182690	-0.440701
11	1	-3.616582	0.970293	0.836081
12	1	-2.181137	1.233680	1.826480
13	1	-2.970183	-0.346391	1.816842
14	1	-0.953317	1.043954	-1.627204
15	1	-0.953596	2.009343	-0.168425
16	1	-2.460246	1.766826	-1.068509
17	1	-2.007982	-1.184936	-1.624273
18	1	-3.522545	-0.471393	-1.090821
19	1	-2.799401	-1.785877	-0.163632
20	1	-0.080435	0.272683	1.185252
21	1	-0.892425	-1.269461	1.358028
22	1	0.298830	-0.650257	-1.349922
23	1	0.234815	-2.183758	-0.493710
24	1	4.322987	-0.505403	-0.314948
25	1	4.217805	1.149867	0.292299
26	1	3.885268	-0.228958	1.351406

ACh + Amide

1	6	-2.001453	2.822840	0.622837
2	6	-0.512980	2.838647	0.863266
3	8	0.069291	1.899914	1.437360
4	6	-2.373196	2.420873	-0.829046
5	6	-1.940379	1.037796	-1.214315
6	6	-0.944368	0.706009	-2.073148
7	6	-2.508951	-0.212142	-0.748897
8	7	-0.835898	-0.666162	-2.173160
9	6	-1.790697	-1.247395	-1.372125
10	6	-3.557261	-0.537930	0.119870
11	6	-2.080370	-2.593233	-1.143625
12	6	-3.848330	-1.866269	0.351800
13	6	-3.113264	-2.886442	-0.276496
14	7	0.165232	3.902236	0.412248
15	6	1.606204	4.042198	0.571203

16	6	-0.448109	-1.191442	2.280381
17	7	1.060926	-1.316178	2.187070
18	6	1.449008	-2.730190	2.506296
19	6	1.668371	-0.364948	3.187891
20	6	1.462283	-0.932816	0.769080
21	6	2.923414	-1.229022	0.435725
22	8	3.336556	-0.417320	-0.683866
23	6	2.966246	-0.728725	-1.950039
24	6	3.659958	0.112104	-2.963919
25	8	2.152168	-1.602445	-2.172197
26	1	-2.435211	2.124016	1.322113
27	1	-1.949005	3.140357	-1.521487
28	1	-3.450425	2.510512	-0.922434
29	1	-0.304130	1.345927	-2.639875
30	1	-0.150935	-1.150789	-2.702028
31	1	-4.141237	0.230265	0.590525
32	1	-1.537949	-3.371833	-1.645245
33	1	-4.658177	-2.129854	1.003866
34	1	-3.375692	-3.910597	-0.093659
35	1	1.879918	4.046488	1.616841
36	1	1.913294	4.975347	0.125528
37	1	2.127829	3.231306	0.082366
38	1	-0.742655	-1.414353	3.293712
39	1	-0.900595	-1.892432	1.599473
40	1	-0.715029	-0.183123	2.017774
41	1	2.522352	-2.820616	2.539634
42	1	1.045266	-3.385746	1.750809
43	1	1.041805	-2.994421	3.469131
44	1	2.742111	-0.445973	3.164055
45	1	1.313895	-0.631431	4.171166
46	1	1.356000	0.634577	2.934646
47	1	0.812633	-1.474662	0.102571
48	1	1.258551	0.121154	0.674842
49	1	3.078007	-2.267116	0.186887
50	1	3.602125	-0.939244	1.218401
51	1	4.723755	-0.085541	-2.931420
52	1	3.281579	-0.112664	-3.947572
53	1	3.517901	1.160268	-2.738481
54	1	-0.333138	4.647774	-0.011942
55	1	-2.415540	3.802446	0.835890

ACh + Ester

1	6	-2.216953	2.611972	0.850796
2	6	-0.739758	2.700577	1.067618
3	8	-0.060985	1.874431	1.668000
4	6	-2.566870	2.322417	-0.630864
5	6	-2.018623	1.019868	-1.134706
6	6	-1.001952	0.853271	-2.017884
7	6	-2.466888	-0.311939	-0.775590
8	7	-0.768235	-0.490844	-2.230281
9	6	-1.661115	-1.221760	-1.482120
10	6	-3.477730	-0.803454	0.059210
11	6	-1.826214	-2.602967	-1.368504
12	6	-3.646638	-2.167601	0.177000
13	6	-2.824848	-3.060521	-0.532716
14	8	-0.199884	3.786118	0.514631
15	6	1.215084	4.077882	0.641056
16	6	-0.377080	-1.404677	2.204030
17	7	1.136556	-1.433058	2.110914
18	6	1.602170	-2.851573	2.274985
19	6	1.687733	-0.568640	3.217034
20	6	1.521183	-0.875664	0.747564
21	6	2.999029	-1.041778	0.398343
22	8	3.347689	-0.108699	-0.645193
23	6	3.021677	-0.354707	-1.939843
24	6	3.654552	0.614324	-2.875776
25	8	2.287345	-1.274282	-2.238558
26	1	-2.603365	1.834623	1.492756
27	1	-2.200701	3.139074	-1.239914
28	1	-3.648022	2.330710	-0.716608
29	1	-0.431123	1.595225	-2.532035
30	1	-0.056625	-0.867649	-2.809066
31	1	-4.128095	-0.133454	0.589027
32	1	-1.218669	-3.283989	-1.933441
33	1	-4.427997	-2.557403	0.799937
34	1	-2.994005	-4.115930	-0.439297
35	1	1.351379	5.013325	0.131466
36	1	1.796212	3.297334	0.176126
37	1	1.479589	4.166053	1.682223
38	1	-0.662183	-1.757635	3.182361
39	1	-0.788425	-2.046137	1.443279
40	1	-0.703811	-0.390620	2.057518
41	1	2.678689	-2.885066	2.308840
42	1	1.238496	-3.439325	1.446934
43	1	1.206483	-3.243341	3.198296
44	1	2.764233	-0.587409	3.195095
45	1	1.344847	-0.960762	4.161434
46	1	1.323527	0.435560	3.076819
47	1	0.909431	-1.379727	0.018177
48	1	1.257351	0.168592	0.762861
49	1	3.223773	-2.041175	0.061064
50	1	3.656826	-0.774407	1.206546
51	1	3.312425	0.429739	-3.880812
52	1	3.417548	1.627493	-2.580725
53	1	4.730953	0.507644	-2.834431
54	1	-2.660864	3.555243	1.142304

(-) Nic

1	6	-0.712854	-0.130382	0.550103
2	6	-1.437896	-1.477457	0.545398
3	7	-1.509071	0.667310	-0.507848
4	6	-2.920618	-1.103876	0.423697
5	6	-2.949690	0.151501	-0.465309
6	6	-1.390600	2.154553	-0.364601
7	6	0.762267	-0.115508	0.255660
8	6	1.291247	-0.757533	-0.860797
9	7	2.587048	-0.758045	-1.142551
10	6	3.436256	-0.138862	-0.322900

11	6	3.007609	0.516855	0.821292
12	6	1.652571	0.531007	1.109595
13	1	-0.908084	0.381042	1.483350
14	1	-1.116842	-2.084752	-0.291641
15	1	-1.220092	-2.030946	1.447164
16	1	-3.509022	-1.901006	-0.005890
17	1	-3.336920	-0.882167	1.397449
18	1	-3.254461	-0.053828	-1.479524
19	1	-3.573021	0.935663	-0.068189
20	1	-1.940867	2.631506	-1.160208
21	1	-0.351088	2.433188	-0.420935
22	1	-1.801479	2.444421	0.589163
23	1	0.673223	-1.296754	-1.552893
24	1	4.470183	-0.176324	-0.592700
25	1	3.712962	0.999955	1.465568
26	1	1.297390	1.029364	1.992070
27	1	-1.117474	0.424003	-1.402811

(-) Nic + Amide

1	6	1.170807	2.197630	-1.633995
2	6	0.330009	2.342097	-0.390984
3	8	-0.319620	1.382385	0.078505
4	6	2.692861	2.245862	-1.347496
5	6	3.175946	1.171739	-0.419353
6	6	3.626688	1.335928	0.848535
7	6	3.276774	-0.246111	-0.709325
8	7	3.990320	0.116976	1.386047
9	6	3.791696	-0.866309	0.441443
10	6	3.007438	-1.026385	-1.840345
11	6	4.029184	-2.238990	0.500863
12	6	3.240951	-2.385722	-1.788234
13	6	3.745687	-2.986475	-0.622731
14	7	0.303769	3.537009	0.197842
15	6	-0.467756	3.815695	1.404019
16	6	-2.432480	-1.335717	0.955781
17	6	-2.188759	-0.682137	2.321591
18	7	-1.059152	-1.222831	0.311466
19	6	-0.752721	-1.095655	2.712607
20	6	-0.082969	-1.572687	1.410145
21	6	-0.879552	-2.024067	-0.929402
22	6	-3.542340	-0.771727	0.108575
23	6	-3.579767	0.571463	-0.257378
24	7	-4.563424	1.089477	-0.984692
25	6	-5.569791	0.308469	-1.377500
26	6	-5.623692	-1.038451	-1.058503
27	6	-4.592787	-1.583091	-0.308699
28	1	0.909621	1.255651	-2.091573
29	1	2.956760	3.217800	-0.944683
30	1	3.203232	2.167962	-2.301743
31	1	3.731132	2.233939	1.416635
32	1	4.415092	-0.010483	2.270941
33	1	2.650046	-0.576162	-2.747482
34	1	4.435122	-2.697422	1.382088
35	1	3.059520	-2.992906	-2.653909
36	1	3.930731	-4.042998	-0.615086
37	1	-0.249774	4.821805	1.725407
38	1	-0.197938	3.128613	2.192113
39	1	-1.528339	3.731398	1.213539
40	1	-2.591669	-2.399121	1.088291
41	1	-2.265588	0.392403	2.233505
42	1	-2.928043	-1.007854	3.038924
43	1	-0.214982	-0.263326	3.141704
44	1	-0.757018	-1.892570	3.443227
45	1	0.853586	-1.087209	1.194335
46	1	0.060408	-2.642798	1.390203
47	1	0.136790	-1.914433	-1.272301
48	1	-1.562543	-1.668710	-1.683530
49	1	-1.079716	-3.062765	-0.714389
50	1	-2.801529	1.248761	0.026658
51	1	-6.339054	0.777114	-1.954347
52	1	-6.445656	-1.641546	-1.385864
53	1	-4.612490	-2.624552	-0.047443
54	1	0.800893	4.288048	-0.218946
55	1	-0.876971	-0.239651	0.087169
56	1	0.912169	2.985357	-2.333818

(-) Nic + Ester

1	6	1.235743	2.213994	-1.620128
2	6	0.418624	2.288837	-0.370020
3	8	-0.318205	1.393361	0.044434
4	6	2.753884	2.280611	-1.328127
5	6	3.232976	1.206376	-0.397012
6	6	3.707781	1.381556	0.861129
7	6	3.288133	-0.219604	-0.659574
8	7	4.045180	0.163466	1.416903
9	6	3.800712	-0.832040	0.497245
10	6	2.978444	-1.015189	-1.769767
11	6	3.993420	-2.210540	0.583039
12	6	3.167022	-2.380323	-1.691005
13	6	3.668194	-2.972576	-0.519588
14	8	0.555184	3.434248	0.277606
15	6	-0.172371	3.723639	1.503314
16	6	-2.471623	-1.448434	0.771400
17	6	-2.092868	-1.044455	2.201379
18	7	-1.147247	-1.268662	0.039634
19	6	-0.651044	-1.562384	2.396846
20	6	-0.100324	-1.821615	0.981917
21	6	-1.097263	-1.863664	-1.324739
22	6	-3.615847	-0.713965	0.124813
23	6	-3.628495	0.673788	0.011447
24	7	-4.638453	1.340018	-0.536011
25	6	-5.697466	0.668887	-0.988968
26	6	-5.779727	-0.712137	-0.915375
27	6	-4.721751	-1.409800	-0.353853
28	1	0.981769	1.296509	-2.129042
29	1	2.985121	3.253485	-0.914921
30	1	3.270781	2.213114	-2.279467
31	1	3.844969	2.288257	1.407987

32	1	4.476283	0.040631	2.299439
33	1	2.629538	-0.571938	-2.683675
34	1	4.398462	-2.663005	1.467735
35	1	2.957236	-2.999184	-2.542042
36	1	3.820197	-4.034071	-0.491691
37	1	0.159667	4.702438	1.793514
38	1	0.074113	2.991938	2.255018
39	1	-1.231695	3.721117	1.305674
40	1	-2.665018	-2.513594	0.736619
41	1	-2.131368	0.031376	2.303638
42	1	-2.788090	-1.464769	2.913475
43	1	-0.046492	-0.837785	2.922118
44	1	-0.636340	-2.475962	2.974606
45	1	0.835054	-1.329855	0.775072
46	1	0.003398	-2.874664	0.768404
47	1	-0.102096	-1.739939	-1.720746
48	1	-1.812221	-1.364122	-1.957588
49	1	-1.333558	-2.914789	-1.262065
50	1	-2.809658	1.270613	0.355841
51	1	-6.485770	1.253829	-1.413687
52	1	-6.643978	-1.224894	-1.284902
53	1	-4.763104	-2.480603	-0.283658
54	1	-0.953230	-0.270959	-0.046900
55	1	0.956920	3.046424	-2.254993

(+) Epi

1	6	-2.034438	-0.697990	1.247918
2	6	-1.259774	0.493911	0.592381
3	6	-2.003218	0.665175	-0.758227
4	6	-3.433946	1.183306	-0.542611
5	6	-4.176585	-0.036259	0.080623
6	6	-3.074988	-1.099249	0.190876
7	7	-2.290056	-0.803437	-1.101307
8	1	-1.451990	-1.352286	-1.203916
9	6	0.235807	0.301982	0.414421
10	6	1.078384	1.420087	0.412840
11	6	2.433818	1.272074	0.203460
12	6	2.915870	-0.012382	-0.007642
13	7	2.147455	-1.070960	-0.000678
14	6	0.837877	-0.929656	0.213879
15	1	-2.525455	-0.399555	2.162315
16	1	-1.411613	1.394827	1.170487
17	1	-1.436919	1.148441	-1.535782
18	1	-3.433189	2.047988	0.104320
19	1	-3.883999	1.484612	-1.479328
20	1	-4.596992	0.179065	1.051381
21	1	-4.986549	-0.373222	-0.553166
22	1	-3.407446	-2.122906	0.223249
23	1	0.676818	2.400820	0.584075
24	1	3.097914	2.109832	0.204955
25	1	0.297741	-1.854068	0.240635
26	1	-2.844084	-0.916377	-1.934579
27	1	-1.382083	-1.520395	1.498234
28	17	4.657248	-0.263059	-0.300381

(+) Epi + Amide

1	6	1.175433	2.791865	-1.333859
2	6	0.281266	2.549269	-0.145378
3	8	0.047025	1.390432	0.263418
4	6	2.652486	3.051514	-0.940496
5	6	3.304845	1.940498	-0.172871
6	6	3.772988	2.006737	1.096947
7	6	3.594531	0.599562	-0.643910
8	7	4.327556	0.797205	1.466511
9	6	4.236348	-0.077967	0.409473
10	6	3.391816	-0.070189	-1.857548
11	6	4.671583	-1.397039	0.287527
12	6	3.813736	-1.380761	-1.982527
13	6	4.451411	-2.037618	-0.915578
14	7	-0.238681	3.611322	0.463323
15	6	-1.141789	3.517030	1.608197
16	6	-0.776050	-1.935110	1.812657
17	6	-1.580117	-2.292797	0.519199
18	6	-0.467485	-2.275437	-0.570383
19	6	0.365393	-3.562850	-0.454675
20	6	1.096887	-3.377496	0.910411
21	6	0.682298	-1.958422	1.342125
22	7	0.533298	-1.278701	-0.008764
23	1	0.232366	-0.299382	0.056525
24	6	-2.793973	-1.433662	0.228315
25	6	-3.980416	-2.022174	-0.213401
26	6	-5.086728	-1.240454	-0.492932
27	6	-4.961513	0.126132	-0.316634
28	7	-3.860507	0.700766	0.099811
29	6	-2.793589	-0.054561	0.373236
30	1	1.108735	1.921329	-1.969363
31	1	2.711516	3.967775	-0.363171
32	1	3.198501	3.236839	-1.860018
33	1	3.764748	2.830696	1.775718
34	1	4.793695	0.623833	2.322483
35	1	2.943647	0.430250	-2.694816
36	1	5.182112	-1.892008	1.091242
37	1	3.690267	-1.894584	-2.916258
38	1	4.795794	-3.044747	-1.049504
39	1	-2.094415	3.098423	1.315139
40	1	-1.299574	4.509160	2.000466
41	1	-0.704809	2.900204	2.378686
42	1	-0.948676	-2.645981	2.607575
43	1	-1.929595	-3.313972	0.591497
44	1	-0.794587	-2.007579	-1.560144
45	1	-0.258579	-4.443461	-0.485477
46	1	1.074307	-3.636331	-1.269654
47	1	0.793655	-4.106389	1.648092
48	1	2.168472	-3.452695	0.794559
49	1	1.381771	-1.435767	1.970926
50	1	-4.046255	-3.086830	-0.333430
51	1	-6.007612	-1.667241	-0.828392
52	1	-1.934263	0.484997	0.701858
53	1	1.396198	-1.268919	-0.531708

54	1	-0.059178	4.513043	0.089592
55	1	0.810237	3.638146	-1.903731
56	1	-1.038492	-0.955576	2.185911
57	17	-6.358471	1.191926	-0.665028

(+) Epi + Ester

1	6	1.105543	2.713065	-1.444972
2	6	0.232095	2.459800	-0.258205
3	8	-0.039829	1.340919	0.177884
4	6	2.553856	3.077905	-1.030441
5	6	3.232795	2.035859	-0.191130
6	6	3.670526	2.189592	1.082527
7	6	3.569186	0.677862	-0.575037
8	7	4.248960	1.020044	1.534479
9	6	4.204131	0.081651	0.530582
10	6	3.415727	-0.066932	-1.751735
11	6	4.677437	-1.229512	0.496861
12	6	3.877503	-1.369883	-1.789976
13	6	4.506155	-1.944838	-0.671348
14	8	-0.217435	3.562999	0.310669
15	6	-1.143644	3.535838	1.438158
16	6	-0.773128	-2.203504	1.741051
17	6	-1.601811	-2.421578	0.431968
18	6	-0.501777	-2.344687	-0.666749
19	6	0.329730	-3.637836	-0.650007
20	6	1.103504	-3.537208	0.700025
21	6	0.677775	-2.163122	1.247317
22	7	0.503680	-1.384524	-0.049212
23	1	0.184267	-0.422007	0.071376
24	6	-2.779646	-1.490034	0.219960
25	6	-3.940264	-1.961511	-0.398842
26	6	-5.008540	-1.112841	-0.621203
27	6	-4.874645	0.202621	-0.210461
28	7	-3.799614	0.665562	0.376865
29	6	-2.771424	-0.157179	0.598442
30	1	1.101921	1.823633	-2.057197
31	1	2.535322	4.020257	-0.497035
32	1	3.114179	3.249385	-1.943574
33	1	3.625097	3.052345	1.709765
34	1	4.698698	0.910014	2.409561
35	1	2.980551	0.372900	-2.628997
36	1	5.181754	-1.661625	1.339745
37	1	3.797945	-1.938094	-2.696818
38	1	4.884918	-2.946364	-0.738776
39	1	-2.057546	3.047341	1.141769
40	1	-1.316722	4.569568	1.669901
41	1	-0.687399	3.023970	2.269462
42	1	-0.922627	-3.003616	2.451193
43	1	-1.990439	-3.431006	0.419582
44	1	-0.839047	-2.009522	-1.632364
45	1	-0.300004	-4.512693	-0.712718
46	1	1.012002	-3.667187	-1.489949
47	1	0.839954	-4.323647	1.392090
48	1	2.171886	-3.579757	0.544856
49	1	1.381804	-1.682802	1.904230
50	1	-4.014736	-2.989048	-0.700598
51	1	-5.908700	-1.451039	-1.088149
52	1	-1.933837	0.297658	1.074615
53	1	1.361657	-1.329209	-0.579134
54	1	0.684320	3.528439	-2.015835
55	1	-1.037182	-1.280851	2.236190
56	17	-6.219270	1.352522	-0.479838

(-) Epi

1	6	1.251069	0.515279	-0.510780
2	6	1.910293	1.186578	0.751372
3	6	3.043482	0.227408	1.136100
4	6	4.169413	0.256651	0.094328
5	6	3.519915	-0.411416	-1.153218
6	6	2.098885	-0.761529	-0.681940
7	7	2.381962	-1.118335	0.789096
8	1	1.546816	-1.296234	1.323485
9	6	-0.243698	0.303147	-0.348963
10	6	-1.096318	1.413960	-0.375691
11	6	-2.455211	1.251267	-0.212310
12	6	-2.931658	-0.039458	-0.020076
13	7	-2.152933	-1.088494	0.000766
14	6	-0.836660	-0.932724	-0.165350
15	1	1.407095	1.135403	-1.383392
16	1	2.300368	2.171382	0.540243
17	1	1.191842	1.284734	1.553811
18	1	3.352329	0.258840	2.167197
19	1	4.488941	1.271223	-0.091088
20	1	5.035447	-0.295822	0.434605
21	1	3.486755	0.242622	-2.011598
22	1	4.058027	-1.302029	-1.450184
23	1	1.631822	-1.575678	-1.206643
24	1	-0.698945	2.399171	-0.530846
25	1	-3.127649	2.082079	-0.234255
26	1	-0.285268	-1.850475	-0.159817
27	1	3.001552	-1.905213	0.894973
28	17	-4.680554	-0.307482	0.208450

(-) Epi + Amide

1	6	-2.312078	-2.569977	-1.752684
2	6	-0.823997	-2.331239	-1.717673
3	8	-0.359067	-1.176182	-1.588889
4	6	-2.877222	-3.022534	-0.381189
5	6	-2.599653	-2.074718	0.747521
6	6	-1.814817	-2.313736	1.826679
7	6	-3.124752	-0.733610	0.915554
8	7	-1.798400	-1.212873	2.658843
9	6	-2.600137	-0.233527	2.122086
10	6	-3.998255	0.068749	0.170260
11	6	-2.913232	1.040208	2.595612
12	6	-4.308185	1.334888	0.631151
13	6	-3.768642	1.814848	1.837933
14	7	-0.028504	-3.392462	-1.812197

15	6	1.431504	-3.316118	-1.767757
16	6	1.345565	2.390701	-0.729186
17	6	0.894322	2.143978	-2.207775
18	6	-0.636730	2.189740	-2.124779
19	6	-1.132037	3.586130	-1.708479
20	6	-0.762733	3.657534	-0.194642
21	6	-0.007903	2.337160	0.035174
22	7	-0.845741	1.413856	-0.835780
23	1	-0.548596	0.439581	-0.929476
24	6	2.425683	1.472575	-0.196402
25	6	3.533948	1.999754	0.467901
26	6	4.507439	1.159912	0.979265
27	6	4.328468	-0.200482	0.806473
28	7	3.299153	-0.718512	0.182655
29	6	2.363242	0.092168	-0.317985
30	1	-2.778632	-1.646338	-2.060763
31	1	-2.476270	-3.999371	-0.133944
32	1	-3.947291	-3.156231	-0.502366
33	1	-1.263318	-3.192657	2.077660
34	1	-1.337457	-1.169520	3.533922
35	1	-4.448691	-0.298805	-0.732236
36	1	-2.524026	1.399020	3.529040
37	1	-4.999203	1.947731	0.085167
38	1	-4.049789	2.789253	2.187818
39	1	1.799881	-2.663982	-2.546048
40	1	1.827047	-4.306668	-1.926771
41	1	1.777605	-2.948997	-0.813618
42	1	1.718981	3.401577	-0.637320
43	1	1.279907	2.894323	-2.882492
44	1	1.221282	1.177141	-2.563815
45	1	-1.153376	1.732391	-2.950753
46	1	-0.650198	4.355947	-2.293634
47	1	-2.198981	3.685087	-1.858108
48	1	-0.148663	4.511089	0.050658
49	1	-1.649174	3.702896	0.423466
50	1	0.043428	1.991502	1.052310
51	1	3.642773	3.061215	0.583771
52	1	5.367787	1.539151	1.487921
53	1	1.562474	-0.402768	-0.822280
54	1	-1.809179	1.387962	-0.537010
55	1	-0.440008	-4.286534	-1.940333
56	1	-2.549192	-3.320464	-2.498085
57	17	5.548181	-1.341092	1.455968

(-) Epi + Ester

1	6	-2.360309	-2.429270	-1.903391
2	6	-0.886736	-2.224119	-1.752187
3	8	-0.347641	-1.118973	-1.667458
4	6	-2.997613	-2.953216	-0.591844
5	6	-2.715226	-2.091659	0.604176
6	6	-1.991053	-2.444302	1.695153
7	6	-3.154748	-0.728221	0.832154
8	7	-1.933081	-1.395072	2.590291
9	6	-2.644886	-0.333984	2.083762
10	6	-3.945415	0.172394	0.106867
11	6	-2.890258	0.929524	2.620366
12	6	-4.189170	1.428667	0.631359
13	6	-3.664261	1.802008	1.881756
14	8	-0.202578	-3.350528	-1.693060
15	6	1.250526	-3.383418	-1.540141
16	6	1.444082	2.453390	-0.626975
17	6	0.982539	2.323771	-2.117393
18	6	-0.548508	2.364821	-2.025068
19	6	-1.038670	3.733781	-1.523073
20	6	-0.647869	3.719675	-0.013420
21	6	0.092472	2.380319	0.138554
22	7	-0.757019	1.514035	-0.780984
23	1	-0.459500	0.551407	-0.922769
24	6	2.493416	1.465271	-0.160139
25	6	3.570974	1.896990	0.615650
26	6	4.508830	0.990383	1.075709
27	6	4.327069	-0.339918	0.741503
28	7	3.327799	-0.767383	0.009726
29	6	2.428862	0.109829	-0.444203
30	1	-2.799579	-1.486426	-2.192641
31	1	-2.635589	-3.956633	-0.408568
32	1	-4.066626	-3.032020	-0.758599
33	1	-1.512386	-3.373404	1.912829
34	1	-1.509224	-1.434264	3.484193
35	1	-4.387963	-0.113678	-0.828399
36	1	-2.514417	1.207237	3.586330
37	1	-4.822283	2.114669	0.102152
38	1	-3.895992	2.770747	2.280404
39	1	1.711199	-2.868433	-2.366595
40	1	1.498303	-4.427671	-1.552229
41	1	1.535198	-2.926223	-0.608387
42	1	1.847085	3.443667	-0.464157
43	1	1.363076	3.126407	-2.731973
44	1	1.310893	1.391917	-2.555654
45	1	-1.070609	1.959145	-2.874372
46	1	-0.566188	4.536007	-2.070886
47	1	-2.107729	3.838765	-1.651509
48	1	-0.018229	4.550676	0.267283
49	1	-1.524838	3.744841	0.618794
50	1	0.141431	1.977290	1.134639
51	1	3.683160	2.936646	0.857499
52	1	5.345295	1.296836	1.666612
53	1	1.653386	-0.314825	-1.042116
54	1	-1.720570	1.474515	-0.481163
55	1	-2.531728	-3.147612	-2.693870
56	17	5.496942	-1.564761	1.321705